Supplementary Information

Accurate Band Gaps for Semiconductors from Density Functional Theory

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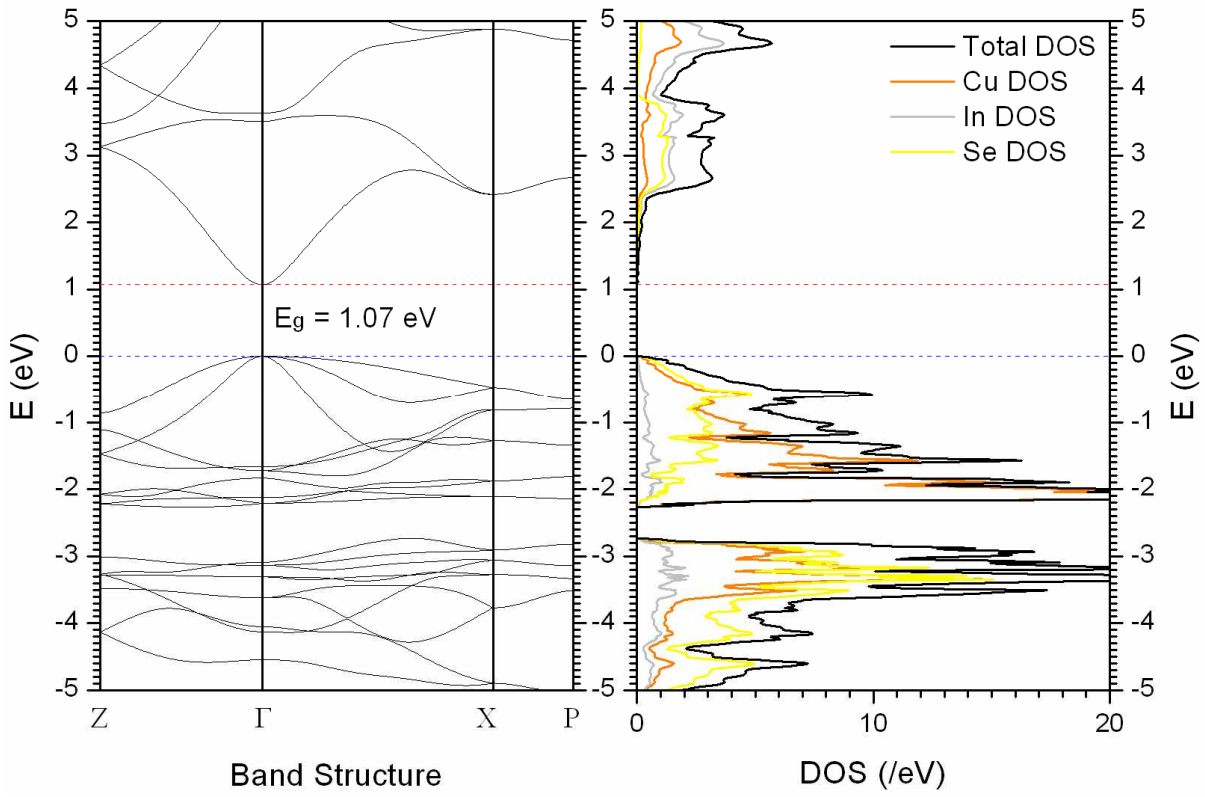

Figure S1. The band structure and density of states (DOS) of $CuInSe_2$ calculated with B3PW91.

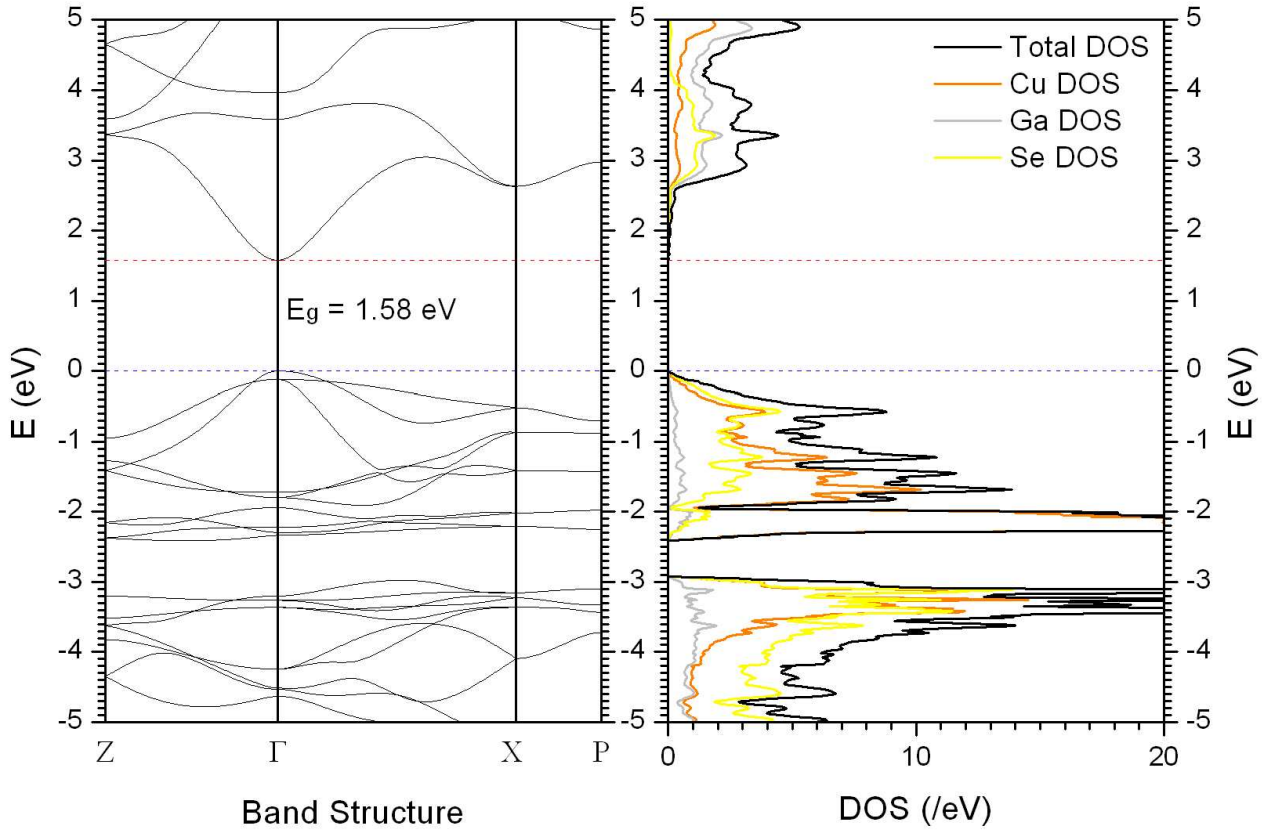

Figure S2. The band structure and density of states (DOS) of $CuGaSe_2$ calculated with B3PW91.

Table S1. Band gaps (eV) for 27 semiconductors. Experimental references quoted next to the band gap. B3LYP leads to MAD = 0.19 eV.

Species	*Exptl.*	B3LYP	Species	*Exptl.*	B3LYP	Species	*Exptl.*	B3LYP
InP	1.42	1.32	$CuAlS_2$	3.46	3.37	$AgAlSe_2$	2.55	2.52
InAs	0.41	0.00	$CuGaS_2$	2.50	2.26	$AgGaSe_2$	1.82	1.50
InSb	0.23	0.00	$CuInS_2$	1.55	1.47	$AgInSe_2$	1.24	1.15
ZnS	3.84	3.53	$CuAlSe_2$	2.65	2.47	$CuAlTe_2$	2.06	2.09
ZnSe	2.83	2.52	$CuGaSe_2$	1.67	1.40	$CuGaTe_2$	1.25	1.12

ZnTe	2.39	2.01	$CuInSe_2$	1.04	0.95	$CuInTe_2$	1.00	0.99
CdS	2.58	2.36	$AgAlS_2$	3.60	3.40	$AgAlTe_2$	2.35	1.98
CdSe	1.85	1.68	$AgGaS_2$	2.70	2.43	$AgGaTe_2$	1.36	1.02
CdTe	1.61	1.47	$AgInS_2$	1.87	1.76	$AgInTe_2$	1.04	0.94

Table S2. Lattice parameters (in Å) for 9 binary semiconductors. B3LYP leads to MAD = 3.1%.

Species	*Exptl.*	B3LYP	Species	*Exptl.*	B3LYP	Species	*Exptl.*	B3LYP
InP	5.869	6.015	ZnS	5.345	5.520	CdS	5.811	6.004
InAs	6.058	6.245	ZnSe	5.669	5.820	CdSe	6.077	6.289
InSb	6.479	6.681	ZnTe	6.103	6.290	CdTe	6.483	6.726

Table S3. Lattice parameter results for 18 ternary semiconductors (X = S, Se, Te). The MAD for B3LYP is 3.6%.

Species	***Exptl.***				**B3LYP**				
	a / Å	**c / Å**	**η = c/2a**	**u(X)**	**a / Å**	**c / Å**	**η = c/2a**	**u(X)**	**% error volume**
$CuAlS_2$	5.334	10.444	0.979	0.268	5.462	10.628	0.973	0.268	6.74
$CuGaS_2$	5.347	10.474	0.979	0.254	5.494	10.731	0.977	0.260	8.13
$CuInS_2$	5.523	11.133	1.008	0.229	5.686	11.453	1.007	0.234	9.03
$CuAlSe_2$	5.606	10.901	0.972	0.257	5.785	11.258	0.973	0.264	9.99
$CuGaSe_2$	5.614	11.022	0.982	0.259	5.812	11.371	0.978	0.257	10.56
$CuInSe_2$	5.781	11.642	1.007	0.226	5.998	12.046	1.004	0.232	11.40
$AgAlS_2$	5.695	10.260	0.901	0.300	5.893	10.499	0.891	0.304	9.58
$AgGaS_2$	5.757	10.304	0.895	0.291	5.922	10.648	0.899	0.296	9.35
$AgInS_2$	5.876	11.201	0.953	0.264	6.077	11.590	0.954	0.270	10.67
$AgAlSe_2$	5.956	10.750	0.902	0.270	6.182	11.166	0.903	0.295	11.90
$AgGaSe_2$	5.992	10.883	0.908	0.288	6.206	11.299	0.910	0.288	11.36
$AgInSe_2$	6.104	11.712	0.959	0.258	6.357	12.181	0.958	0.264	12.81
$CuAlTe_2$	5.976	11.804	0.988	0.250	6.239	12.299	0.986	0.251	13.57

$CuGaTe_2$	6.023	11.940	0.991	0.256	6.241	12.359	0.990	0.247	11.13
$CuInTe_2$	6.194	12.416	1.002	0.222	6.433	12.897	1.002	0.226	12.02
$AgAlTe_2$	6.296	11.830	0.939	0.260	6.568	12.367	0.942	0.277	13.75
$AgGaTe_2$	6.288	11.940	0.949	0.260	6.570	12.442	0.947	0.274	13.75
$AgInTe_2$	6.467	12.633	0.977	0.262	6.726	13.155	0.978	0.253	12.64